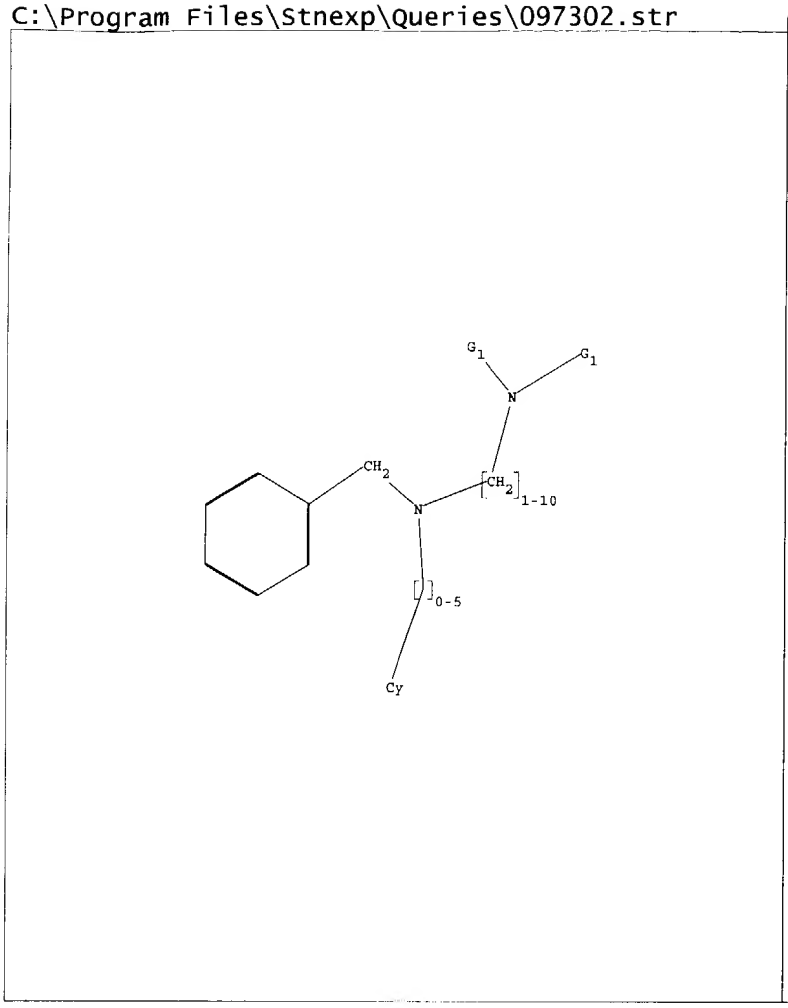
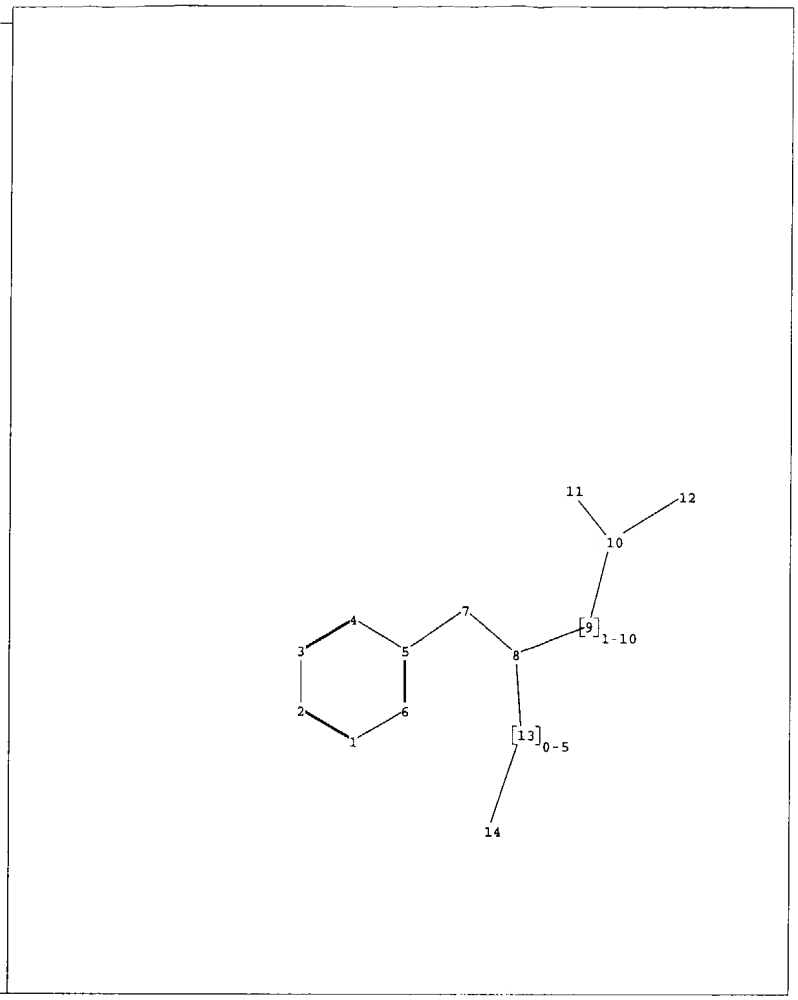
C:\Program Files\Stnexp\Queries\097302.str



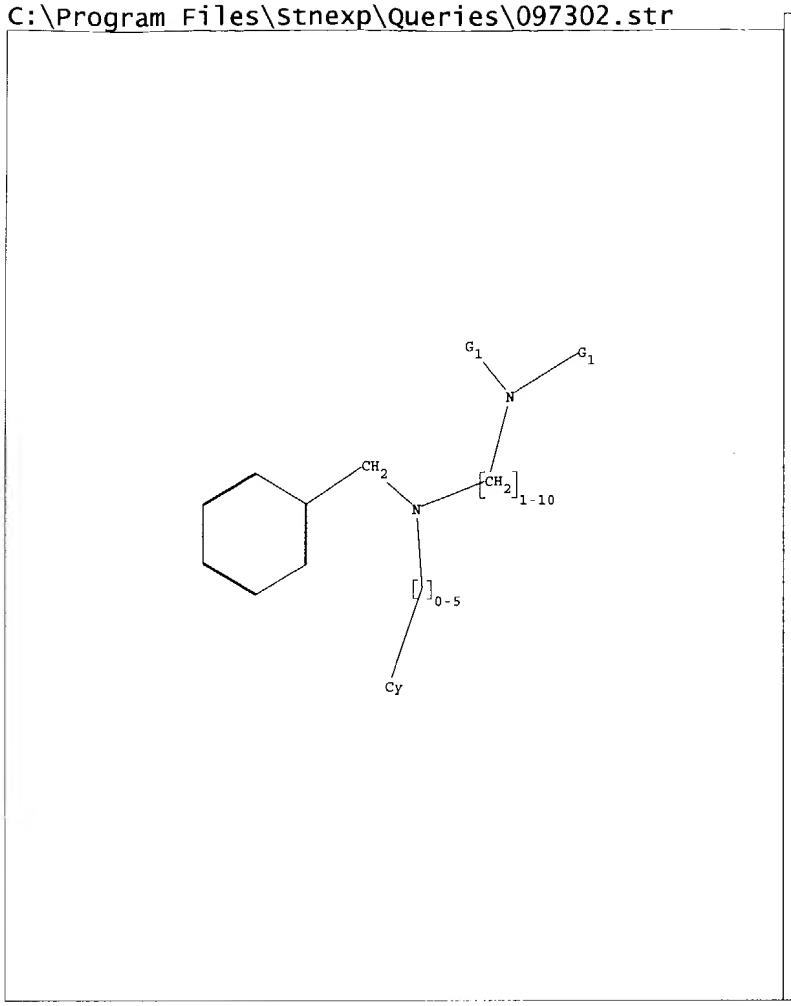


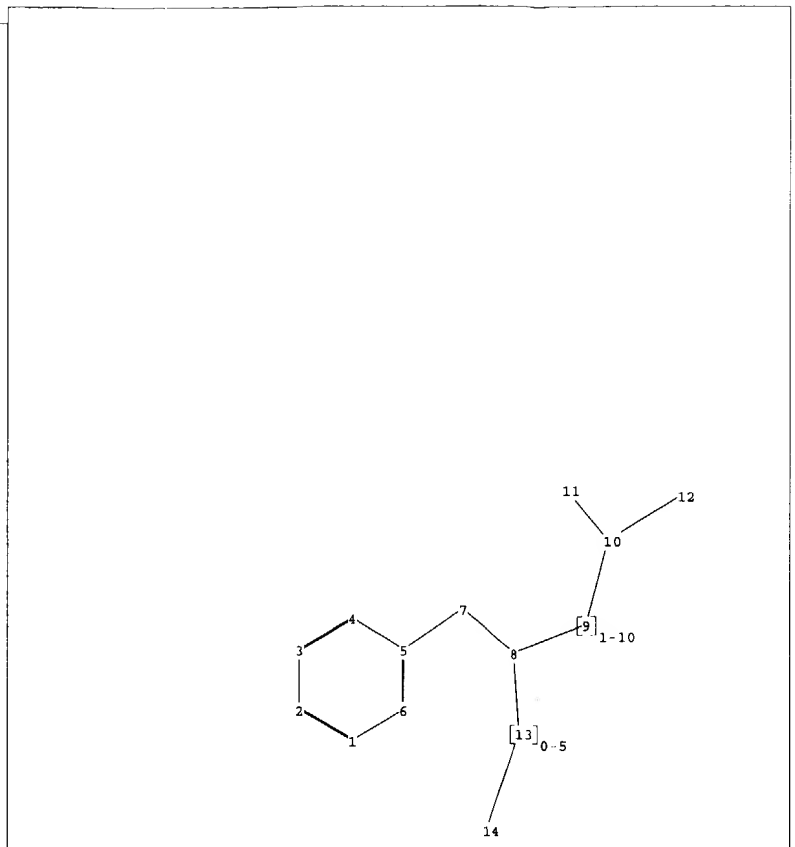
chain nodes :
7 8 9 10 11 12 13 14
ring nodes :
1 2 3 4 5 6
chain bonds :
5-7 7-8 8-9 8-13 9-10 10-11 10-12 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
8-13 10-11 10-12 13-14
exact bonds :
5-7 7-8 8-9 9-10
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

G1:n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:Atom
Generic attributes :
14:
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic

C:\Program Files\Stnexp\Queries\097302.str





chain nodes :
7 8 9 10 11 12 13 14
ring nodes :
1 2 3 4 5 6
chain bonds :
5-7 7-8 8-9 8-13 9-10 10-11 10-12 13-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
8-13 10-11 10-12 13-14
exact bonds :
5-7 7-8 8-9 9-10
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

G1:n-Pr,i-Pr,n-Bu,i-Bu,s-Bu,t-Bu

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:Atom
Generic attributes :
14:
Number of Carbon Atoms : less than 7
Type of Ring System : Monocyclic

765

=> d his

(FILE 'HOME' ENTERED AT 08:19:48 ON 05 AUG 2004)

FILE 'REGISTRY' ENTERED AT 08:20:06 ON 05 AUG 2004
L1 STRUCTURE UPLOADED
L2 9 S L1
L3 1151 S L1 FUL
L4 STRUCTURE UPLOADED
L5 121 SEARCH L4 SSS SUB=L3 FULL
L6 0 SEARCH L4 CSS SUB=L3 FULL

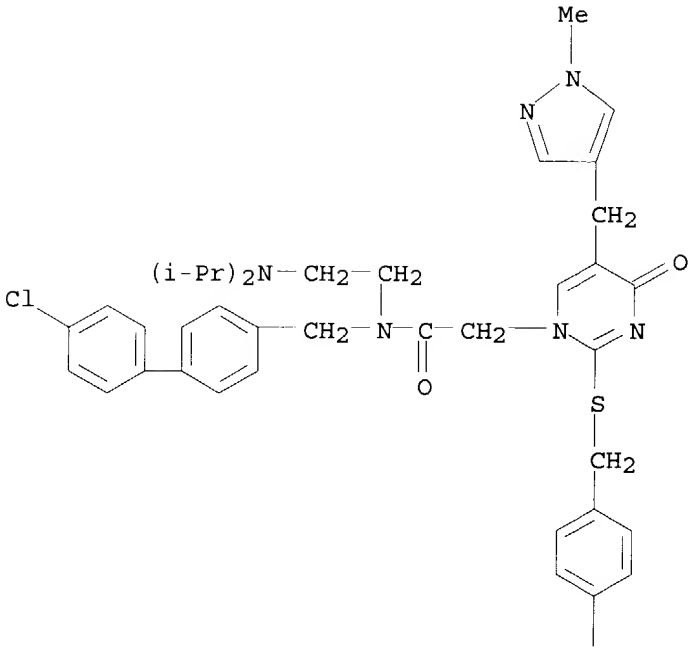
FILE 'CAPLUS' ENTERED AT 08:28:03 ON 05 AUG 2004

=> s l5
L7 13 L5

=> d bib abs hitstr 1-13

L7 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:641070 CAPLUS
DN 138:280725
TI The discovery of SB-435495: A potent, orally active inhibitor of lipoprotein-associated phospholipase A2 for evaluation in man
AU Blackie, Josie A.; Bloomer, Jackie C.; Brown, Murray J. B.; Cheng, Hung-Yuan; Elliott, Richard L.; Hammond, Beverley; Hickey, Deirdre M. B.; Ife, Robert J.; Leach, Colin A.; Lewis, V. Ann; Macphee, Colin H.; Milliner, Kevin J.; Moores, Kitty E.; Pinto, Ivan L.; Smith, Stephen A.; Stansfield, Ian G.; Stanway, Steven J.; Taylor, Maxine A.; Theobald, Colin J.; Whittaker, Caroline M.
CS GlaxoSmithKline, Medicines Research Centre, Stevenage, SG1 2NY, UK
SO Bioorganic & Medicinal Chemistry Letters (2002), 12(18), 2603-2606
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science Ltd.
DT Journal
LA English
AB The introduction of a functionalized amido substituent into a series of 1-(biphenylmethylacetamido)-pyrimidones has given a series of inhibitors of recombinant lipoprotein-associated phospholipase A2 with sub-nanomolar potency and very encouraging developability properties. Diethylaminoethyl derivative, SB-435495, was selected for progression to man.
IT **503534-69-8P**
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(pyrimidone SB-435495 as a lipoprotein-associated phospholipase A2 inhibitor)
RN 503534-69-8 CAPLUS
CN 1(4H)-Pyrimidineacetamide, N-[2-[bis(1-methylethyl)amino]ethyl]-N-[(4'-chloro[1,1'-biphenyl]-4-yl)methyl]-2-[[(4-fluorophenyl)methyl]thio]-5-[(1-methyl-1H-pyrazol-4-yl)methyl]-4-oxo- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:368443 CAPLUS
DN 136:369504
TI Preparation of substituted alkyldiamines as inhibitors of plasmodium falciparum protease plasmepsin II or related aspartic proteases
IN Boss, Christoph; Fischli, Walter; Meyer, Solange; Richard-Bildstein, Sylvia; Weller, Thomas
PA Actelion Pharmaceuticals Ltd., Switz.
SO PCT Int. Appl., 69 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002038534	A2	20020516	WO 2001-EP12617	20011031
	WO 2002038534	A3	20021114		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,

DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
AU 2002014035 A5 20020521 AU 2002-14035 20011031
BR 2001015276 A 20030812 BR 2001-15276 20011031
EP 1335899 A2 20030820 EP 2001-982452 20011031
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
JP 2004513161 T2 20040430 JP 2002-541072 20011031
NO 2003002085 A 20030509 NO 2003-2085 20030509
US 2004067927 A1 20040408 US 2003-416363 20031107
PRAI WO 2000-EP11142 W 20001110
WO 2001-EP12617 W 20011031
OS MARPAT 136:369504

AB Compds. R4(CH)tR3NQANR1R2 [Q = SO2R5, COR5, CONHR5, CONR5R6, CO2R5, (CH2)pR5, (CH2)pCHR5R6; R1, R2 = Pr, pentyl, hexyl, ω-hydroxypropyl, etc., or R1NR2 = ring; R3 = alkyl, alkenyl, aryl, heteroaryl, cycloalkyl, etc.; R4 = H, CH2OR7, CO2R7, alkyl, R5, R6 = alkyl, alkenyl, aryl, cycloalkyl, etc.; R7 = H, alkyl, cycloalkyl, aryl, etc.; t = 0, 1; p = 0-2; A = (CH2)n and n = 2, 3, 4, 5], useful as inhibitors of the plasmodium falciparum protease plasmepsin II or related aspartic proteases, were prepared E.g., reaction of 4-PhCH2OC6H4CH2NHCH2CH2NBu2 with 4-pentylbenzoyl chloride gave 4-PhCH2OC6H4CH2N(CH2CH2NBu2)COC6H4CH2Bu-4 (I). The IC50 value for I on plasmepsin II was 115.

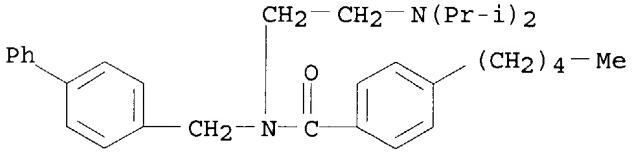
IT **422524-11-6P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(nod preparation of substituted alkyldiamines as inhibitors of plasmodium falciparum protease plasmepsin II or related aspartic proteases)

RN 422524-11-6 CAPLUS

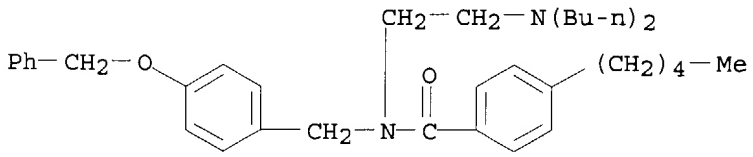
CN Benzamide, N-([1,1'-biphenyl]-4-ylmethyl)-N-[2-[bis(1-methylethyl)amino]ethyl]-4-pentyl- (9CI) (CA INDEX NAME)



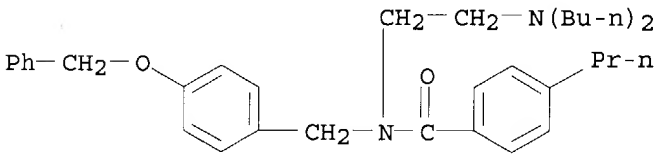
IT **422523-63-5P 422523-64-6P 422523-65-7P**
422523-66-8P 422523-67-9P 422523-68-0P
422523-69-1P 422523-70-4P 422523-71-5P
422523-72-6P 422523-73-7P 422523-74-8P
422523-75-9P 422523-76-0P 422523-77-1P
422523-78-2P 422523-79-3P 422523-82-8P
422523-83-9P 422523-84-0P 422523-85-1P
422523-86-2P 422523-87-3P 422523-88-4P
422523-89-5P 422523-90-8P 422523-91-9P
422523-92-0P 422523-94-2P 422523-95-3P
422523-96-4P 422523-97-5P 422523-98-6P
422523-99-7P 422524-00-3P 422524-01-4P
422524-02-5P 422524-10-5P 422524-14-9P
422524-15-0P 422524-16-1P 422524-17-2P
422524-18-3P 422524-19-4P 422524-20-7P
422524-21-8P 422524-22-9P 422524-23-0P
422524-24-1P 422524-25-2P 422524-26-3P
422524-27-4P 422524-28-5P 422524-29-6P
422524-30-9P 422524-31-0P 422524-33-2P
422524-34-3P 422524-35-4P 422524-36-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted alkyldiamines as inhibitors of plasmodium falciparum protease plasmepsin II or related aspartic proteases)

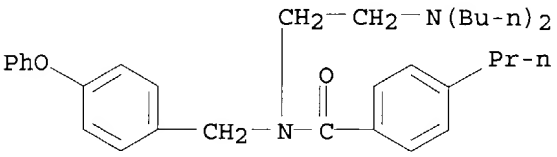
RN 422523-63-5 CAPLUS
CN Benzamide, N-[2-(dibutylamino)ethyl]-4-pentyl-N-[[4-(phenylmethoxy)phenyl]methyl]- (9CI) (CA INDEX NAME)



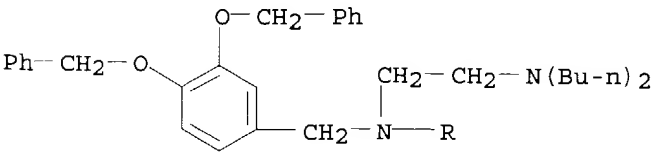
RN 422523-64-6 CAPLUS
CN Benzamide, N-[2-(dibutylamino)ethyl]-N-[[4-(phenylmethoxy)phenyl]methyl]-4-propyl- (9CI) (CA INDEX NAME)

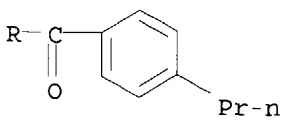


RN 422523-65-7 CAPLUS
CN Benzamide, N-[2-(dibutylamino)ethyl]-N-[(4-phenoxyphenyl)methyl]-4-propyl- (9CI) (CA INDEX NAME)



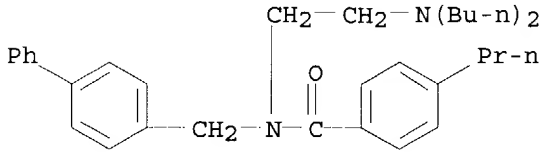
RN 422523-66-8 CAPLUS
CN Benzamide, N-[[3,4-bis(phenylmethoxy)phenyl]methyl]-N-[2-(dibutylamino)ethyl]-4-propyl- (9CI) (CA INDEX NAME)



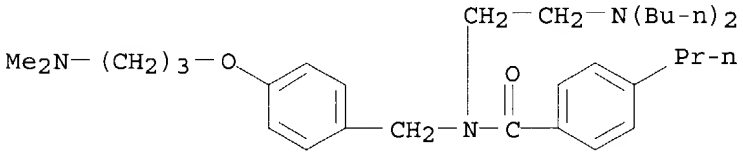


765

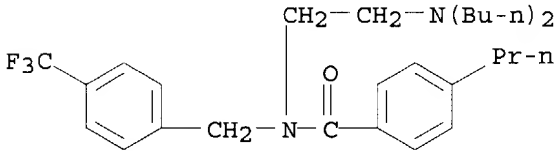
RN 422523-67-9 CAPLUS
CN Benzamide, N-([1,1'-biphenyl]-4-ylmethyl)-N-[2-(dibutylamino)ethyl]-4-propyl- (9CI) (CA INDEX NAME)



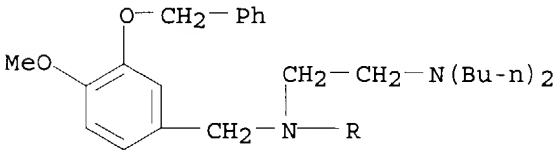
RN 422523-68-0 CAPLUS
CN Benzamide, N-[2-(dibutylamino)ethyl]-N-[[4-[3-(dimethylamino)propoxy]phenyl]methyl]-4-propyl- (9CI) (CA INDEX NAME)

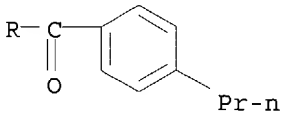


RN 422523-69-1 CAPLUS
CN Benzamide, N-[2-(dibutylamino)ethyl]-4-propyl-N-[[4-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

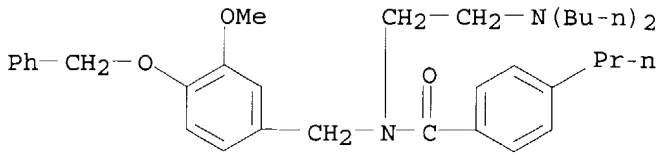


RN 422523-70-4 CAPLUS
CN Benzamide, N-[2-(dibutylamino)ethyl]-N-[[4-methoxy-3-(phenylmethoxy)phenyl]methyl]-4-propyl- (9CI) (CA INDEX NAME)

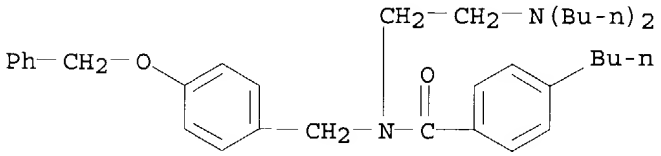




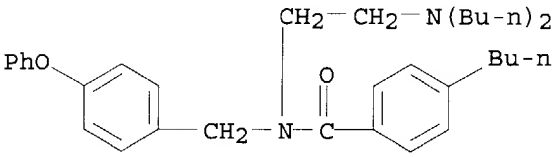
RN 422523-71-5 CAPLUS
CN Benzamide, N-[2-(dibutylamino)ethyl]-N-[[3-methoxy-4-(phenylmethoxy)phenyl]methyl]-4-propyl- (9CI) (CA INDEX NAME)



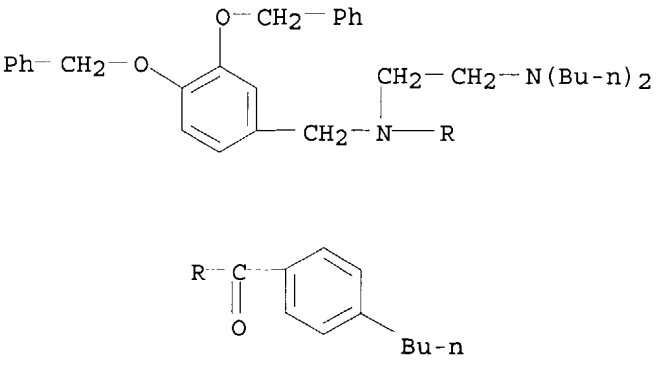
RN 422523-72-6 CAPLUS
CN Benzamide, 4-butyl-N-[2-(dibutylamino)ethyl]-N-[[4-(phenylmethoxy)phenyl]methyl]- (9CI) (CA INDEX NAME)



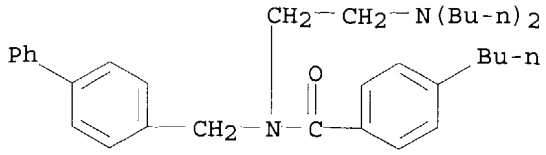
RN 422523-73-7 CAPLUS
CN Benzamide, 4-butyl-N-[2-(dibutylamino)ethyl]-N-[(4-phenoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



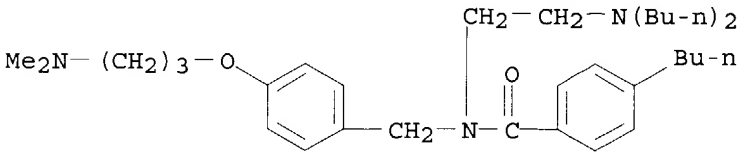
RN 422523-74-8 CAPLUS
CN Benzamide, N-[[3,4-bis(phenylmethoxy)phenyl]methyl]-4-butyl-N-[2-(dibutylamino)ethyl]- (9CI) (CA INDEX NAME)



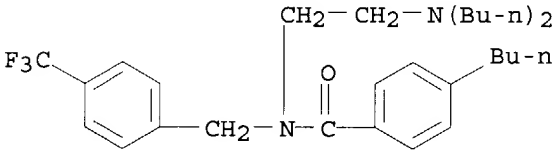
RN 422523-75-9 CAPLUS
CN Benzamide, N-([1,1'-biphenyl]-4-ylmethyl)-4-butyl-N-[2-(dibutylamino)ethyl]- (9CI) (CA INDEX NAME)



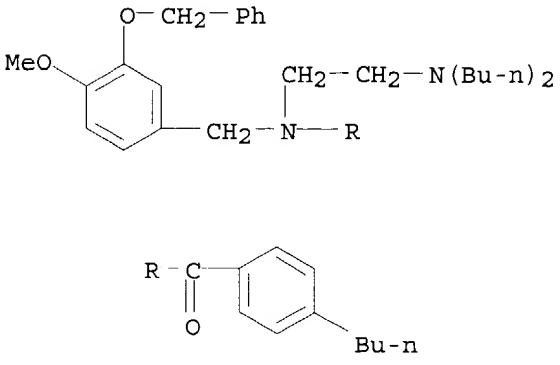
RN 422523-76-0 CAPLUS
CN Benzamide, 4-butyl-N-[2-(dibutylamino)ethyl]-N-[[4-[3-(dimethylamino)propoxy]phenyl]methyl]- (9CI) (CA INDEX NAME)



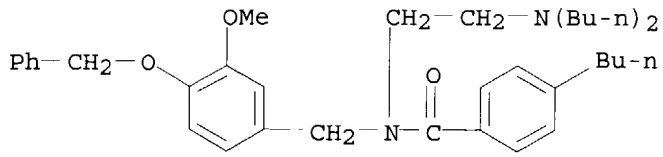
RN 422523-77-1 CAPLUS
CN Benzamide, 4-butyl-N-[2-(dibutylamino)ethyl]-N-[[4-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



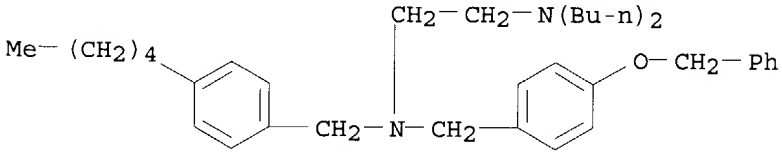
RN 422523-78-2 CAPLUS
CN Benzamide, 4-butyl-N-[2-(dibutylamino)ethyl]-N-[[4-methoxy-3-(phenylmethoxy)phenyl]methyl]- (9CI) (CA INDEX NAME)



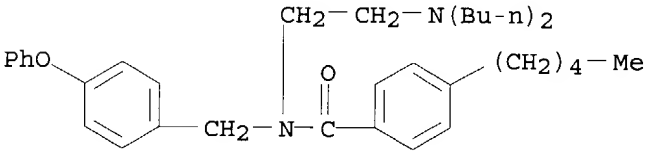
RN 422523-79-3 CAPLUS
CN Benzamide, 4-butyl-N-[2-(dibutylamino)ethyl]-N-[[3-methoxy-4-(phenylmethoxy)phenyl]methyl]- (9CI) (CA INDEX NAME)



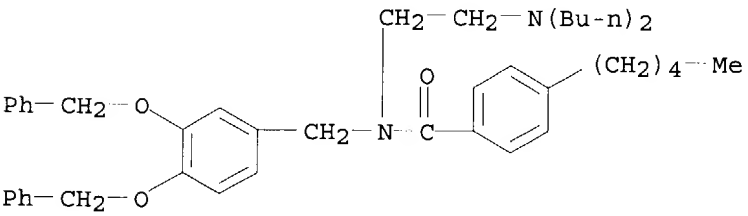
RN 422523-82-8 CAPLUS
CN 1,2-Ethanediamine, N,N-dibutyl-N'-[(4-pentylphenyl)methyl]-N'-[[4-(phenylmethoxy)phenyl]methyl]- (9CI) (CA INDEX NAME)



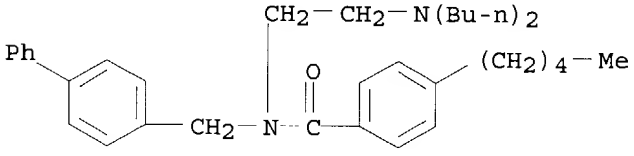
RN 422523-83-9 CAPLUS
CN Benzamide, N-[2-(dibutylamino)ethyl]-4-pentyl-N-[(4-phenoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



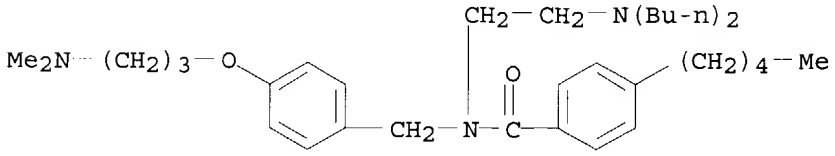
RN 422523-84-0 CAPLUS
CN Benzamide, N-[[3,4-bis(phenylmethoxy)phenyl]methyl]-N-[2-(dibutylamino)ethyl]-4-pentyl- (9CI) (CA INDEX NAME)



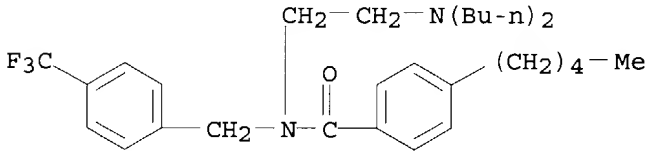
RN 422523-85-1 CAPLUS
CN Benzamide, N-([1,1'-biphenyl]-4-ylmethyl)-N-[2-(dibutylamino)ethyl]-4-pentyl- (9CI) (CA INDEX NAME)



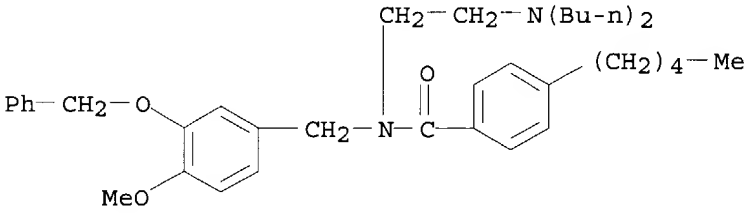
RN 422523-86-2 CAPLUS
CN Benzamide, N-[2-(dibutylamino)ethyl]-N-[[4-[3-(dimethylamino)propoxy]phenyl]methyl]-4-pentyl- (9CI) (CA INDEX NAME)



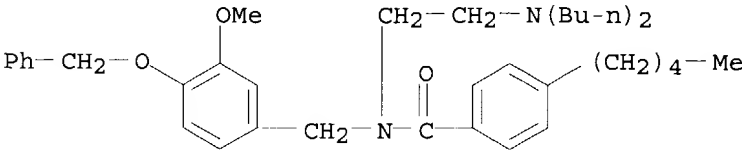
RN 422523-87-3 CAPLUS
CN Benzamide, N-[2-(dibutylamino)ethyl]-4-pentyl-N-[[4-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



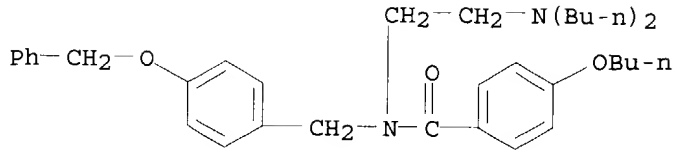
RN 422523-88-4 CAPLUS
CN Benzamide, N-[2-(dibutylamino)ethyl]-N-[[4-methoxy-3-(phenylmethoxy)phenyl]methyl]-4-pentyl- (9CI) (CA INDEX NAME)



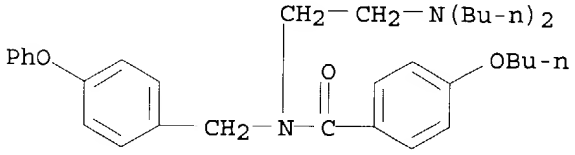
RN 422523-89-5 CAPLUS
CN Benzamide, N-[2-(dibutylamino)ethyl]-N-[[3-methoxy-4-(phenylmethoxy)phenyl]methyl]-4-pentyl- (9CI) (CA INDEX NAME)



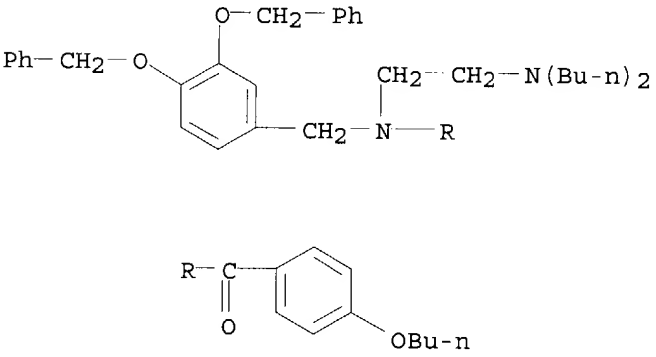
RN 422523-90-8 CAPLUS
CN Benzamide, 4-butoxy-N-[2-(dibutylamino)ethyl]-N-[[4-(phenylmethoxy)phenyl]methyl]- (9CI) (CA INDEX NAME)



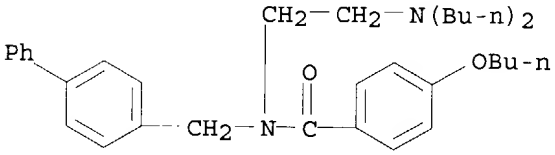
RN 422523-91-9 CAPLUS
CN Benzamide, 4-butoxy-N-[2-(dibutylamino)ethyl]-N-[(4-phenoxyphenyl)methyl]- (9CI) (CA INDEX NAME)



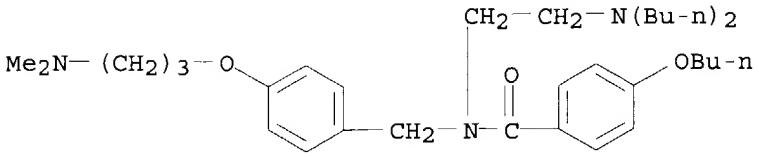
RN 422523-92-0 CAPLUS
CN Benzamide, N-[[3,4-bis(phenylmethoxy)phenyl]methyl]-4-butoxy-N-[2-(dibutylamino)ethyl]- (9CI) (CA INDEX NAME)



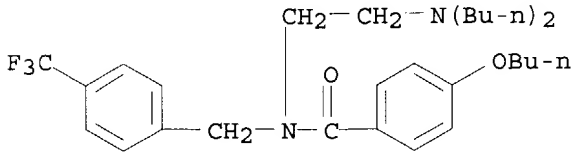
RN 422523-94-2 CAPLUS
CN Benzamide, N-([1,1'-biphenyl]-4-ylmethyl)-4-butoxy-N-[2-(dibutylamino)ethyl]- (9CI) (CA INDEX NAME)



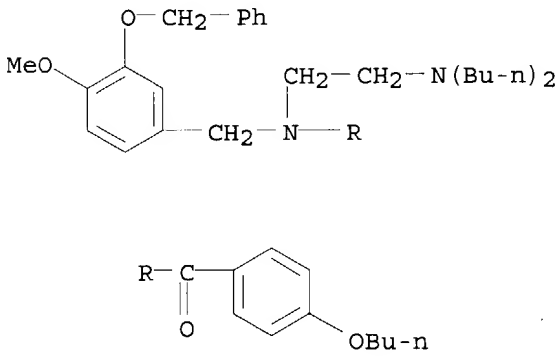
RN 422523-95-3 CAPLUS
CN Benzamide, 4-butoxy-N-[2-(dibutylamino)ethyl]-N-[[4-[3-(dimethylamino)propoxy]phenyl]methyl]- (9CI) (CA INDEX NAME)



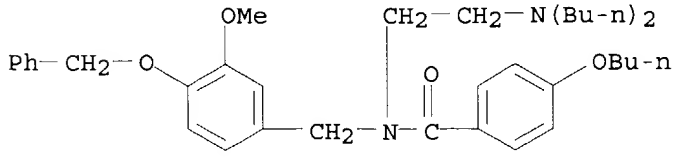
RN 422523-96-4 CAPLUS
CN Benzamide, 4-butoxy-N-[2-(dibutylamino)ethyl]-N-[[4-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



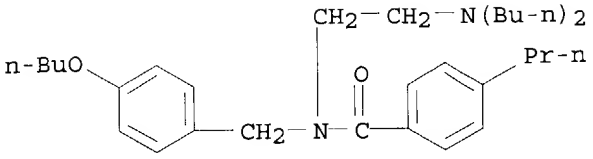
RN 422523-97-5 CAPLUS
CN Benzamide, 4-butoxy-N-[2-(dibutylamino)ethyl]-N-[[4-methoxy-3-(phenylmethoxy)phenyl]methyl]- (9CI) (CA INDEX NAME)



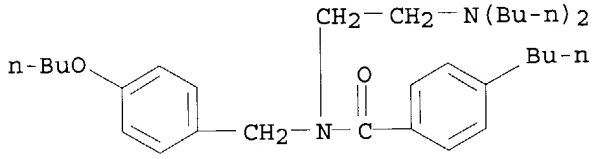
RN 422523-98-6 CAPLUS
CN Benzamide, 4-butoxy-N-[2-(dibutylamino)ethyl]-N-[[3-methoxy-4-(phenylmethoxy)phenyl]methyl]- (9CI) (CA INDEX NAME)



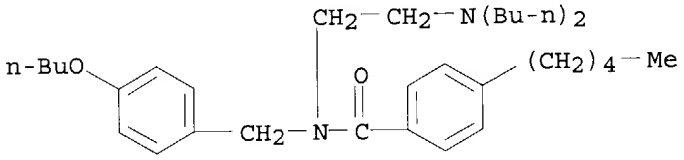
RN 422523-99-7 CAPLUS
CN Benzamide, N-[(4-butoxyphenyl)methyl]-N-[2-(dibutylamino)ethyl]-4-propyl- (9CI) (CA INDEX NAME)



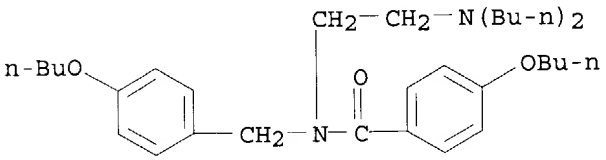
RN 422524-00-3 CAPLUS
CN Benzamide, N-[(4-butoxyphenyl)methyl]-4-butyl-N-[2-(dibutylamino)ethyl]- (9CI) (CA INDEX NAME)



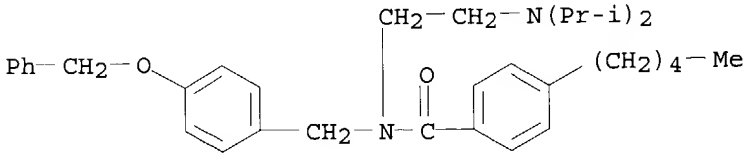
RN 422524-01-4 CAPLUS
CN Benzamide, N-[(4-butoxyphenyl)methyl]-N-[2-(dibutylamino)ethyl]-4-pentyl- (9CI) (CA INDEX NAME)



RN 422524-02-5 CAPLUS
CN Benzamide, 4-butoxy-N-[(4-butoxyphenyl)methyl]-N-[2-(dibutylamino)ethyl]- (9CI) (CA INDEX NAME)

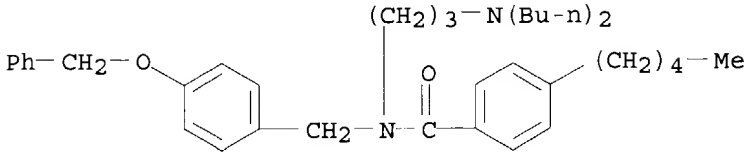


RN 422524-10-5 CAPLUS
CN Benzamide, N-[2-[bis(1-methylethyl)amino]ethyl]-4-pentyl-N-[[4-(phenylmethoxy)phenyl]methyl]- (9CI) (CA INDEX NAME)

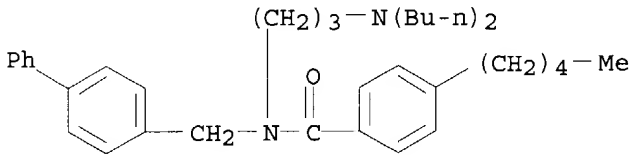


RN 422524-14-9 CAPLUS
CN Benzamide, N-[3-(dibutylamino)propyl]-4-pentyl-N-[[4-

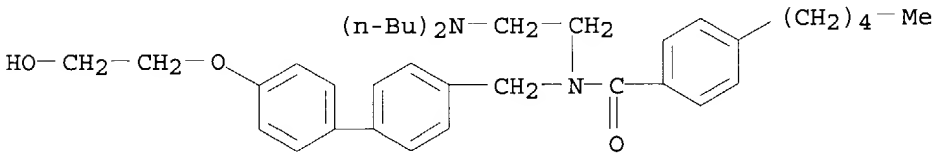
(phenylmethoxy)phenyl]methyl]- (9CI) (CA INDEX NAME)



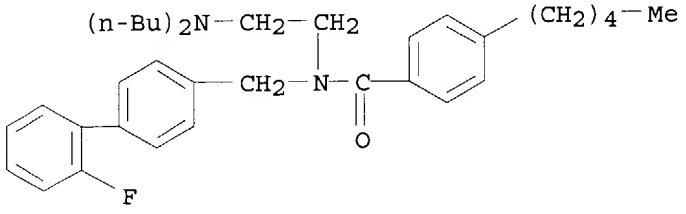
RN 422524-15-0 CAPLUS
CN Benzamide, N-([1,1'-biphenyl]-4-ylmethyl)-N-[3-(dibutylamino)propyl]-4-pentyl- (9CI) (CA INDEX NAME)



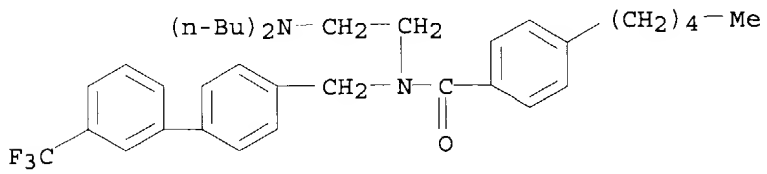
RN 422524-16-1 CAPLUS
CN Benzamide, N-[2-(dibutylamino)ethyl]-N-[[4'-(2-hydroxyethoxy)[1,1'-biphenyl]-4-yl]methyl]-4-pentyl- (9CI) (CA INDEX NAME)



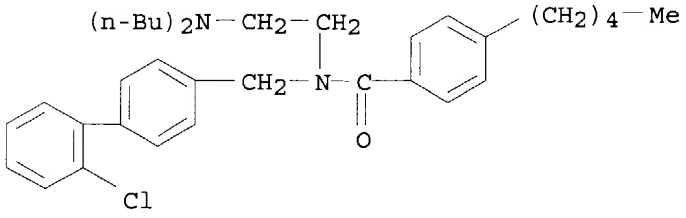
RN 422524-17-2 CAPLUS
CN Benzamide, N-[2-(dibutylamino)ethyl]-N-[(2'-fluoro[1,1'-biphenyl]-4-yl)methyl]-4-pentyl- (9CI) (CA INDEX NAME)



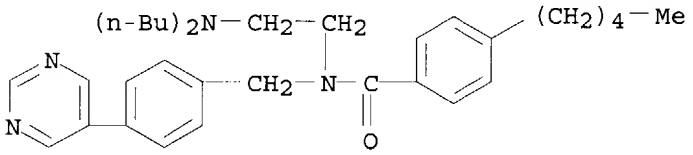
RN 422524-18-3 CAPLUS
CN Benzamide, N-[2-(dibutylamino)ethyl]-4-pentyl-N-[[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]methyl]- (9CI) (CA INDEX NAME)



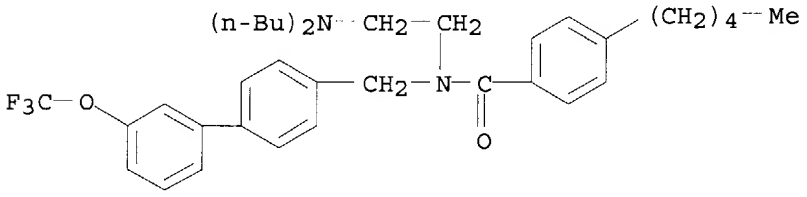
RN 422524-19-4 CAPLUS
CN Benzamide, N-[(2'-chloro[1,1'-biphenyl]-4-yl)methyl]-N-[2-(dibutylamino)ethyl]-4-pentyl- (9CI) (CA INDEX NAME)



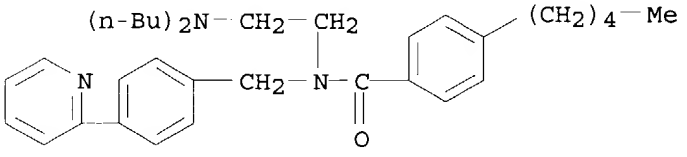
RN 422524-20-7 CAPLUS
CN Benzamide, N-[2-(dibutylamino)ethyl]-4-pentyl-N-[[4-(5-pyrimidinyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



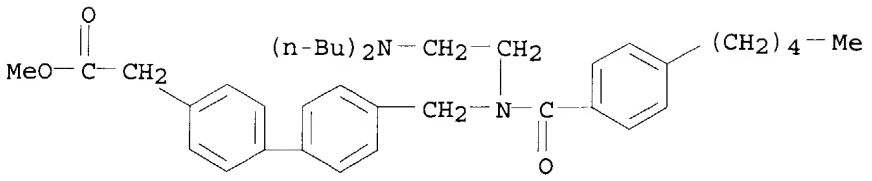
RN 422524-21-8 CAPLUS
CN Benzamide, N-[2-(dibutylamino)ethyl]-4-pentyl-N-[[3'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]methyl]- (9CI) (CA INDEX NAME)



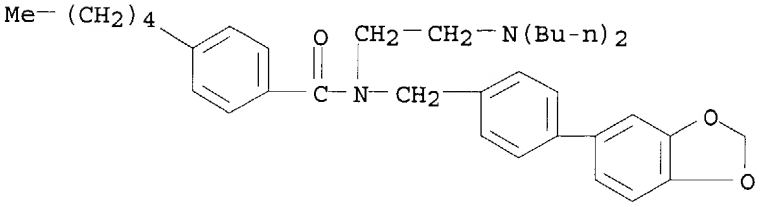
RN 422524-22-9 CAPLUS
CN Benzamide, N-[2-(dibutylamino)ethyl]-4-pentyl-N-[[4-(2-pyridinyl)phenyl]methyl]- (9CI) (CA INDEX NAME)



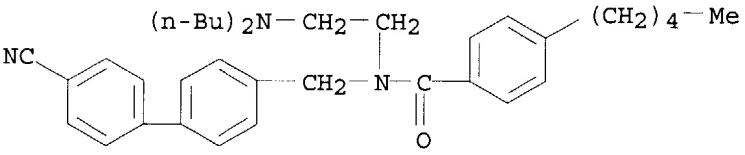
RN 422524-23-0 CAPLUS
CN [1,1'-Biphenyl]-4-acetic acid, 4'-[[[2-(dibutylamino)ethyl](4-pentylbenzoyl)amino]methyl]-, methyl ester (9CI) (CA INDEX NAME)



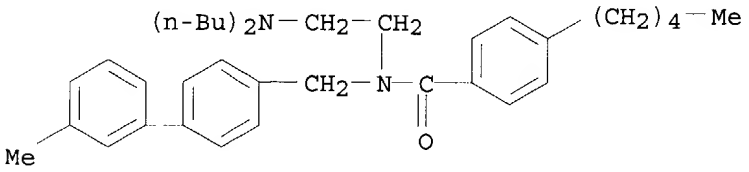
RN 422524-24-1 CAPLUS
CN Benzamide, N-[[4-(1,3-benzodioxol-5-yl)phenyl]methyl]-N-[2-(dibutylamino)ethyl]-4-pentyl- (9CI) (CA INDEX NAME)



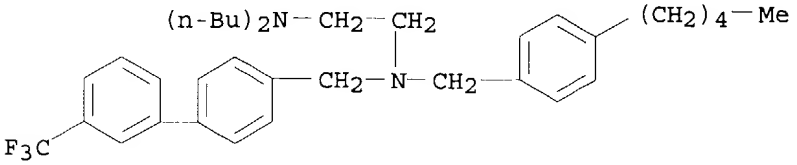
RN 422524-25-2 CAPLUS
CN Benzamide, N-[(4'-cyano[1,1'-biphenyl]-4-yl)methyl]-N-[2-(dibutylamino)ethyl]-4-pentyl- (9CI) (CA INDEX NAME)



RN 422524-26-3 CAPLUS
CN Benzamide, N-[2-(dibutylamino)ethyl]-N-[(3'-methyl[1,1'-biphenyl]-4-yl)methyl]-4-pentyl- (9CI) (CA INDEX NAME)

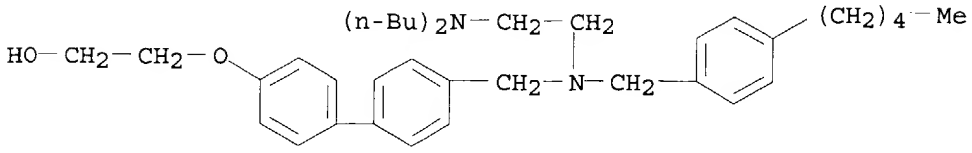


RN 422524-27-4 CAPLUS
CN 1,2-Ethanediamine, N,N-dibutyl-N'-[(4-pentylphenyl)methyl]-N'-[[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]methyl]- (9CI) (CA INDEX NAME)

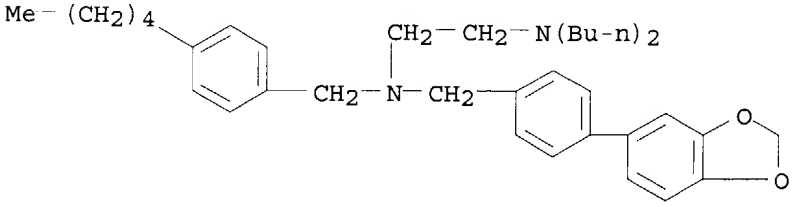


RN 422524-28-5 CAPLUS
CN Ethanol, 2-[[4'-[[[2-(dibutylamino)ethyl][(4-pentylphenyl)methyl]amino]met

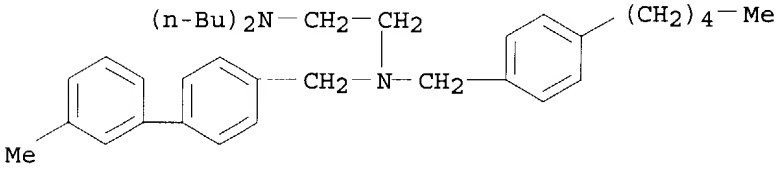
hyl][1,1'-biphenyl]-4-yl]oxy]- (9CI) (CA INDEX NAME)



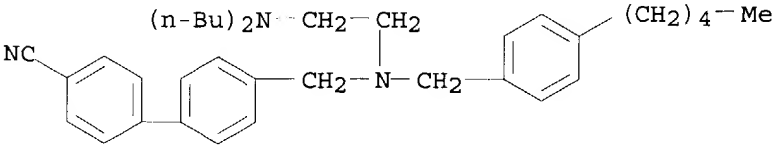
RN 422524-29-6 CAPLUS
CN 1,2-Ethanediamine, N-[[4-(1,3-benzodioxol-5-yl)phenyl]methyl]-N',N'-dibutyl-N-[(4-pentylphenyl)methyl]- (9CI) (CA INDEX NAME)



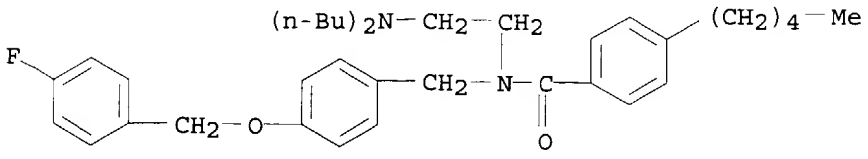
RN 422524-30-9 CAPLUS
CN 1,2-Ethanediamine, N,N-dibutyl-N'-[(3'-methyl[1,1'-biphenyl]-4-yl)methyl]-N'-[(4-pentylphenyl)methyl]- (9CI) (CA INDEX NAME)



RN 422524-31-0 CAPLUS
CN [1,1'-Biphenyl]-4-carbonitrile, 4'-[[[2-(dibutylamino)ethyl][(4-pentylphenyl)methyl]amino]methyl]- (9CI) (CA INDEX NAME)



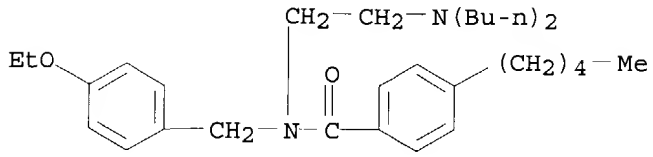
RN 422524-33-2 CAPLUS
CN Benzamide, N-[2-(dibutylamino)ethyl]-N-[[4-[(4-fluorophenyl)methoxy]phenyl]methyl]-4-pentyl- (9CI) (CA INDEX NAME)



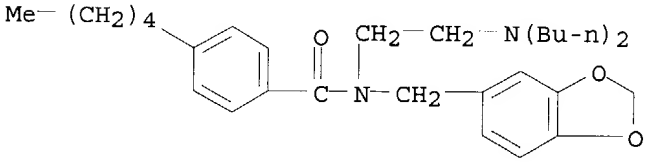
RN 422524-34-3 CAPLUS

765

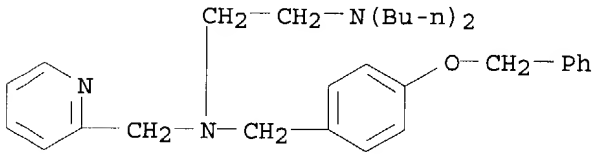
CN Benzamide, N-[2-(dibutylamino)ethyl]-N-[(4-ethoxyphenyl)methyl]-4-pentyl- (9CI) (CA INDEX NAME)



RN 422524-35-4 CAPLUS
CN Benzamide, N-(1,3-benzodioxol-5-ylmethyl)-N-[2-(dibutylamino)ethyl]-4-pentyl- (9CI) (CA INDEX NAME)



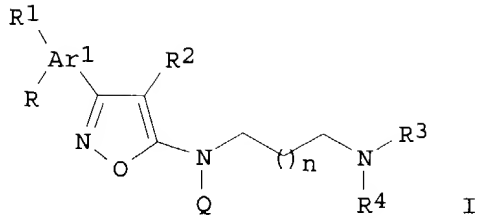
RN 422524-36-5 CAPLUS
CN 1,2-Ethanediamine, N,N-dibutyl-N'-[[4-(phenylmethoxy)phenyl]methyl]-N'-(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)



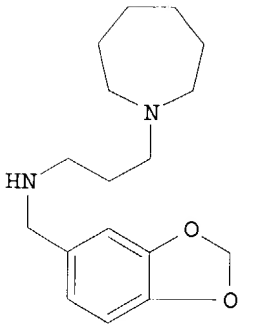
L7 ANSWER 3 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:680066 CAPLUS
DN 135:318498
TI Preparation of aryl-isoxazolyl-amines and use as thrombin receptor antagonists
IN Barrow, James C.; Connolly, Thomas; Freidinger, Roger M.; Nantermet, Philippe G.; Selnick, Harold G.
PA Merck & Co., Inc., USA
SO Brit. UK Pat. Appl., 124 pp.
CODEN: BAXXDU
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 2356198	A1	20010516	GB 2000-26327	20001027
	US 6544982	B1	20030408	US 2000-698811	20001027
PRAI	US 1999-162586P	P	19991029		

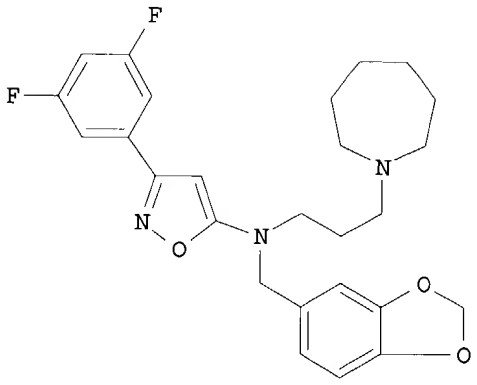
OS MARPAT 135:318498
GI



I



II



III

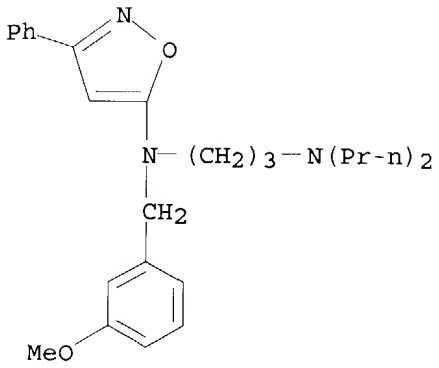
AB Title compds. I [n = 0 - 2; R, R1 = H, alkyl, alkoxy, aryl, halo, CF3, etc. or R, R1 form a 5-membered heterocyclic ring having 1 or 2 heteroatoms; R2 = H, alkyl, alkoxy, halo or CN; R3, R4 = H, alkyl, alkanol, alkenyl, cycloalkyl, etc. or R3 in combination with R4 may form a ring system selected from (un)saturated (un)substituted 4 - 8 membered ring; Q = C(O)alkyl, alkyl, alkyl-cyclo-alkyl or (CH2)m-Ar2(R6)-R5; Ar1-2 = (hetero)aryl; R5, R6 = H, alkyl, alkoxy, CN, OCF3, etc. or R5, R6 form a 5-membered heterocyclic ring having 1 or 2 heteroatoms; m = 0 - 2] were prepared Examples include over 200 synthetic examples and 3 formulations. For instance, Et 3,5-difluorobenzoylacetate was prepared from 3,5-difluoroacetophenone (NaH, EtO2CO, 80°C, 2 h, 85%) and reacted with hydroxylamine (HOAc, reflux, 1 h) to give 3-(3,5-difluorophenyl)-5-chloroisoxazole (35%). III was prepared from this isoxazole and amine II (preparation given) (n-BuLi, Et2O, 0°C, 30 min) and isolated as the HCl salt in 63% yield. I are useful as thrombin inhibitors (no data).

IT **359422-14-3P 359423-78-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug; preparation of aryl-isoxazolyl-amines and use as thrombin receptor antagonists)

RN 359422-14-3 CAPLUS

CN 1,3-Propanediamine, N-[(3-methoxyphenyl)methyl]-N-(3-phenyl-5-isoxazolyl)-N',N'-dipropyl- (9CI) (CA INDEX NAME)

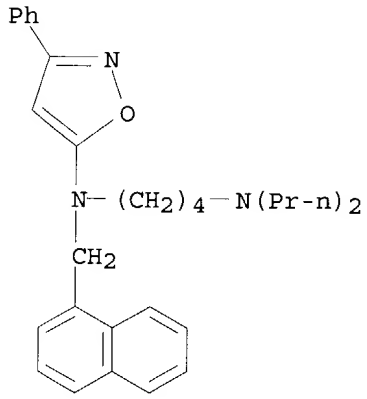
765



RN 359423-78-2 CAPLUS
CN 1,4-Butanediamine, N-(1-naphthalenylmethyl)-N-(3-phenyl-5-isoxazolyl)-N',N'-dipropyl-, trifluoroacetate (9CI) (CA INDEX NAME)

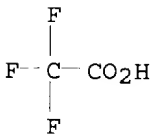
CM 1

CRN 359423-77-1
CMF C30 H37 N3 O



CM 2

CRN 76-05-1
CMF C2 H F3 O2



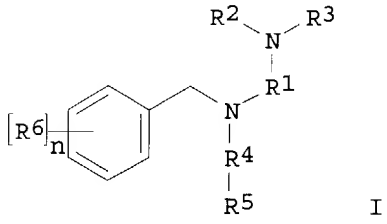
L7 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:416763 CAPLUS
DN 135:33362
TI Preparation of tertiary amino compounds having opioid receptor affinity
IN Kyle, Donald; Goehring, R. Richard; Victory, Sam
PA Euro-Celtique, S.A., Luxembourg

765

SO PCT Int. Appl., 15 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001039767	A1	20010607	WO 2000-US33047	20001206
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 2001041746	A1	20011115	US 2000-730814	20001206
	EP 1244437	A1	20021002	EP 2000-983942	20001206
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2004501060	T2	20040115	JP 2001-541500	20001206
PRAI	US 1999-169396P	P	19991206		
	WO 2000-US33047	W	20001206		

OS MARPAT 135:33362
GI



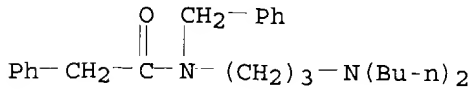
I

AB The title compds. [I; R1 = a bond, alkenylene, etc.; R2, R3 = H, alkyl, alkenyl, etc.; R4 = a bond, alkenylene, etc.; R5 = H, 5-6 membered (hetero)aryl, cycloalkyl; R6 = alkyl, cycloalkyl, halo; n = 0-3], useful for the treatment of chronic and acute pain, were prepared Thus, reacting benzaldehyde with 3-(dibutylamino)propylamine in the presence of NaBH4, 3Å mol. sieves in MeOH followed by amidataion of the resulting I [R1 = (CH2)3; R2, R3 = Bu; R4 = a bond; R5, R6 = H] with phenylacetic acid in the presence of EDCl and DMAP in THF afforded I [R1 = (CH2)3; R2, R3 = Bu; R4 = COCH2; R5 = Ph; R6 = H] which showed Ki of 40 nM against opioid receptor μ binding.

IT **343593-68-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of tertiary amino compds. having opioid receptor affinity)

RN 343593-68-0 CAPLUS

CN Benzeneacetamide, N-[3-(dibutylamino)propyl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



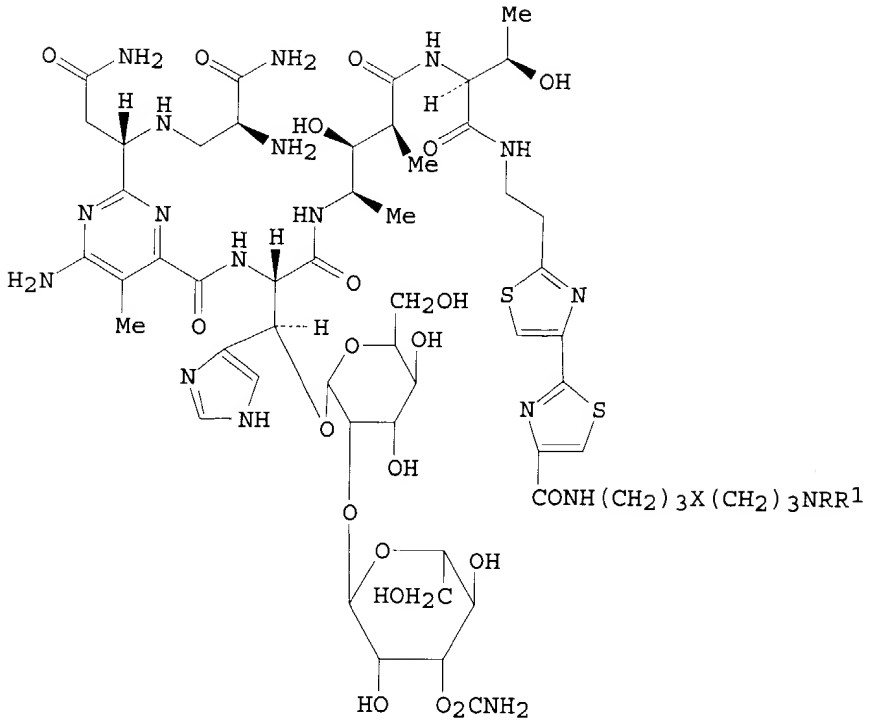
765

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1984:23013 CAPLUS
DN 100:23013
TI Aminopropylaminobleomycin derivatives
IN Umezawa, Hamao; Fujii, Akio; Muraoka, Yasuhiko; Nakatani, Tokuji; Fukuoka, Takeyo; Takahashi, Katsutoshi
PA Microbiochemical Research Foundation, Japan
SO Ger. Offen., 76 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 3247199	A1	19830707	DE 1982-3247199	19821221
	JP 58116497	A2	19830711	JP 1981-210449	19811229
	JP 63006078	B4	19880208		
	CA 1244824	A1	19881115	CA 1982-417731	19821215
	NL 8204857	A	19830718	NL 1982-4857	19821216
	CH 657859	A	19860930	CH 1982-7478	19821222
	GB 2112781	A1	19830727	GB 1982-36626	19821223
	GB 2112781	B2	19851218		
	SE 8207408	A	19830630	SE 1982-7408	19821227
	SE 465034	B	19910715		
	SE 465034	C	19911107		
	ES 518580	A1	19840201	ES 1982-518580	19821227
	AT 8204693	A	19850815	AT 1982-4693	19821227
	AT 380021	B	19860325		
	DK 8205764	A	19830630	DK 1982-5764	19821228
	HU 27462	O	19831028	HU 1982-4179	19821228
	HU 187836	B	19860228		
	CS 237334	B2	19850716	CS 1982-9910	19821228
	IL 67581	A1	19860331	IL 1982-67581	19821228
	FR 2519638	A1	19830718	FR 1982-22035	19821229
	FR 2519638	B1	19851129		
	US 4537880	A	19850827	US 1984-635096	19840727
	US 4568490	A	19860204	US 1985-743738	19850612
PRAI	JP 1981-210449		19811229		
	US 1982-453254		19821227		
	US 1984-635096		19840727		

GI



I

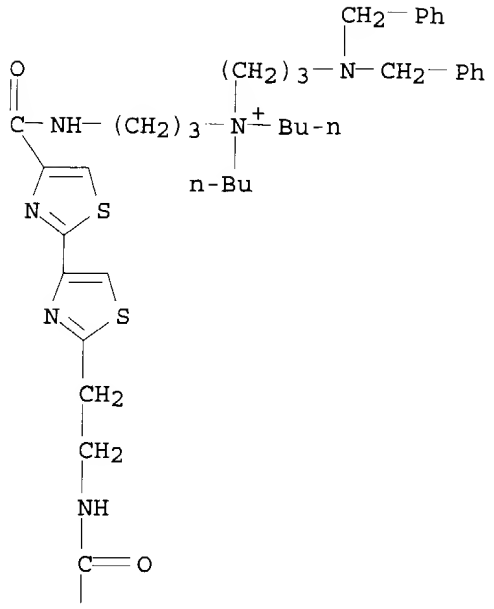
AB Bleomycins I (X = amino, piperazino, aminoalkylamino; NRR1 = amino) (53 compds.) and their Cu chelates were prepared Thus, I (X = NMe, R = R1 = H) was reductively alkylated with cycloundecanecarboxaldehyde to give I Cu chelate (X = NMe, R = cycloundecylmethyl, R1 = H) which was converted to its Cu-free form (II). II caused 50% inhibition of He-La cell growth at 0.58 μg/mL and caused no pulmonary fibrosis in mice at 10 + 5 mg/kg.

IT **88033-80-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and bactericidal and antitumor activity of)

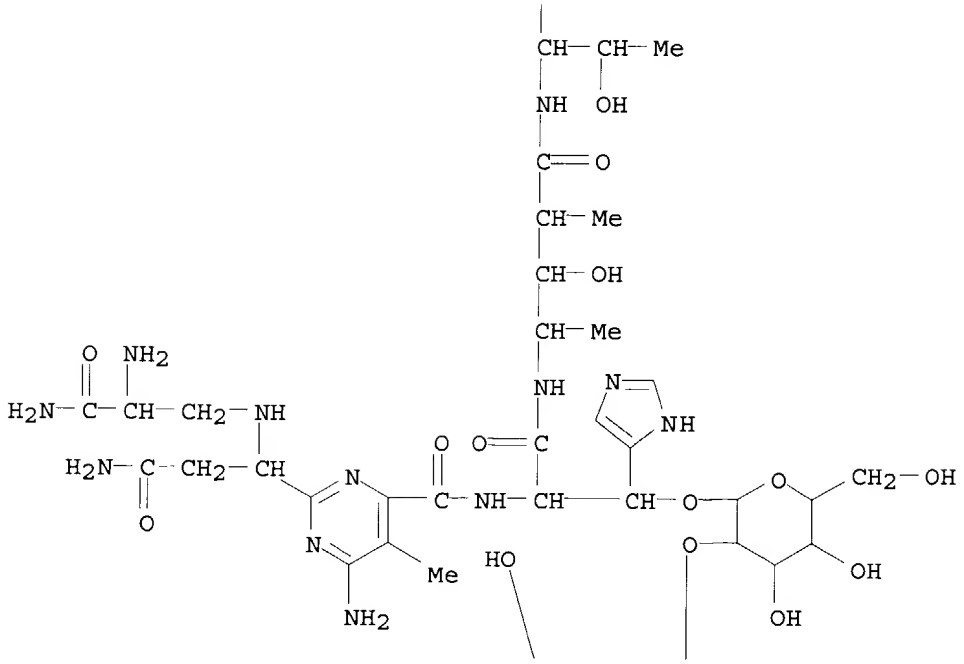
RN 88033-80-1 CAPLUS

CN Bleomycinamide, N1-[3-[[3-[bis(phenylmethyl)amino]propyl]dibutylammonio]propyl]- (9CI) (CA INDEX NAME)

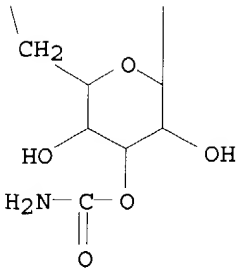
PAGE 1-A



PAGE 2-A

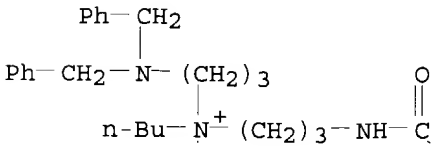


PAGE 3-A

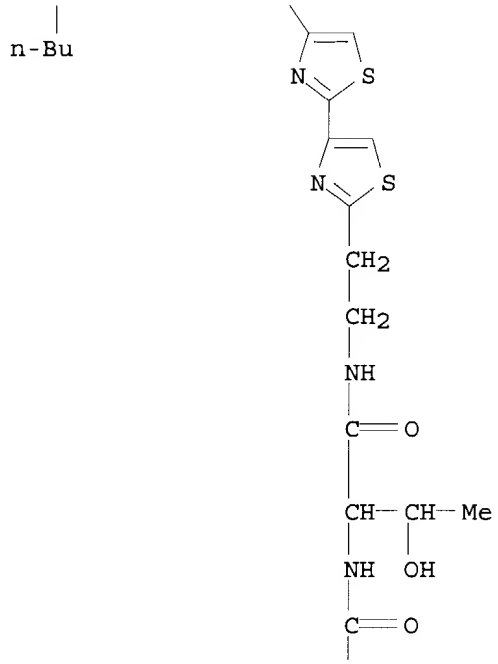


IT **88003-70-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and chromatog. and electrophoresis of)
RN 88003-70-7 CAPLUS
CN Copper(2+), [N1-[3-[[3-[bis(phenylmethyl)amino]propyl]dibutylammonio]propyl]bleomycinamidato]- (9CI) (CA INDEX NAME)

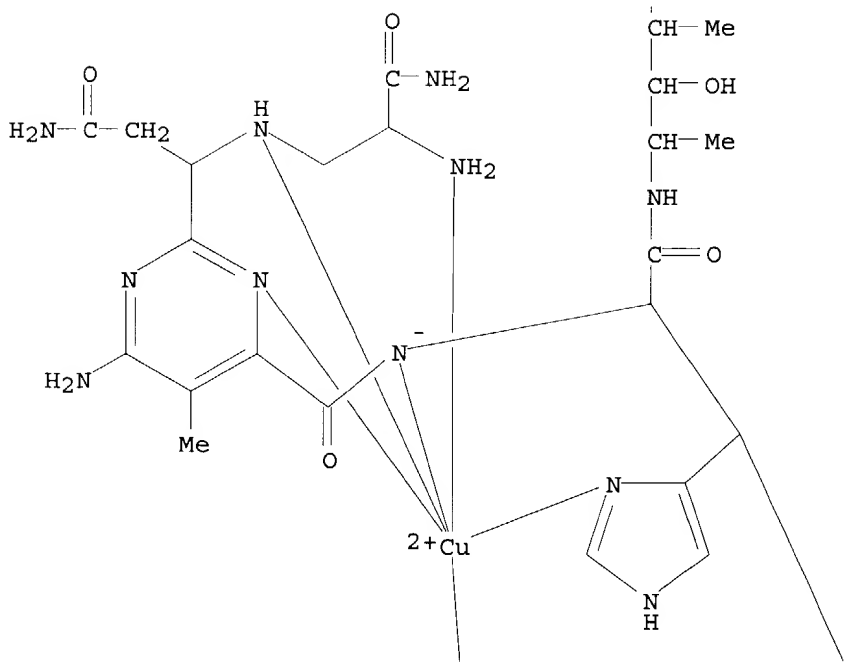
PAGE 1-A



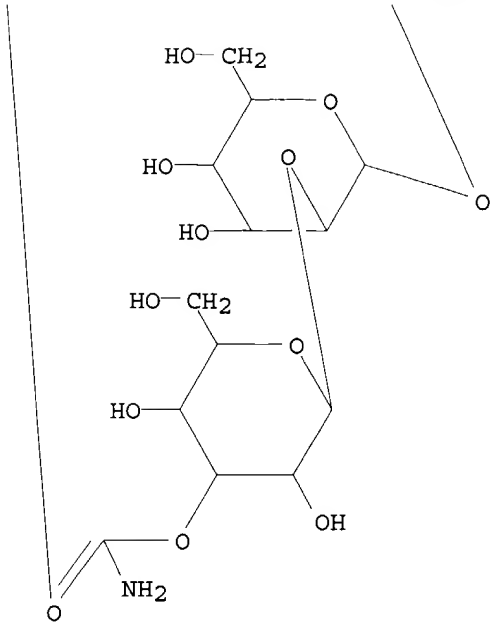
PAGE 2-A



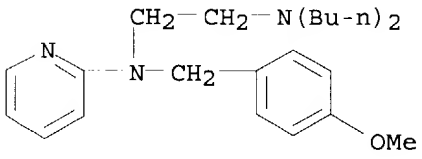
PAGE 3-A



PAGE 4-A



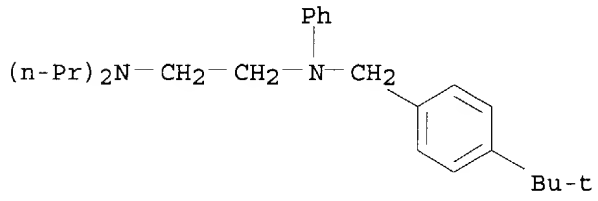
L7 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1982:435554 CAPLUS
DN 97:35554
TI Sources of error in quantitative mass spectrometry
AU Millard, B. J.
CS Lombardy Sci. Comput., Berkhamsted/Berks., UK
SO Comm. Eur. Communities, [Rep.] EUR (1982), EUR 7137, Appl. Mass Spectrom. Trace Anal., 163-79
CODEN: CECED9
DT Report
LA English
AB Sources of error in mass spectroscopy of biol. compds. are discussed with regard to adsorption on glass, decomposition on the gas chromatograph, exchange of label, and internal standard selection.
IT **69569-89-7**
RL: PROC (Process)
(extraction of, from blood plasma, mepyramine compared to)
RN 69569-89-7 CAPLUS
CN 1,2-Ethanediamine, N,N-dibutyl-N'-[(4-methoxyphenyl)methyl]-N'-2-pyridinyl- (9CI) (CA INDEX NAME)



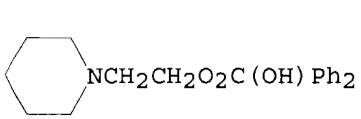
L7 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1979:456187 CAPLUS
DN 91:56187
TI A study of molecular folding in aqueous solution, using the fragmentation constant
AU Tute, M. S.; Canas-Rodriguez, A.

765

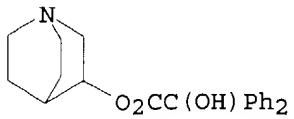
CS Pfizer Cent. Res., Sandwich/Kent, UK
SO Abhandlungen der Akademie der Wissenschaften der DDR, Abteilung Mathematik, Naturwissenschaften, Technik (1978), (2N, Quant. Struct.-Act. Anal.), 53-7
CODEN: AAWTD2; ISSN: 0138-1059
DT Journal
LA English
AB The slope for regression anal. of the logarithm of the partition coefficient (P) of p-Me3CC6H4CH(CH2CH2R)Ph (I; R = NMe2, CH2NMe2, pyrrolidino, piperidino) between n-octanol and an aqueous buffer vs. the hydrophobic fragmental constant (f) is .apprx.1, indicating that aqueous I does not have a folded conformation. The regression anal. of log p vs. f has a slope <1 for p-Me3CC6H4CH2N(CH2CH2R)Ph (II; R = NMe2, NEt2, NPr2, pyrrolidino, piperidino), indicating that aqueous II exists in a folded conformation.
IT **47552-17-0**
RL: PRP (Properties)
(partition coefficient of, between n-octanol and aqueous buffer, folded conformation in relation to hydrophobic fragmental consts. and)
RN 47552-17-0 CAPLUS
CN 1,2-Ethanediamine, N-[[4-(1,1-dimethylethyl)phenyl]methyl]-N-phenyl-N',N'-dipropyl- (9CI) (CA INDEX NAME)



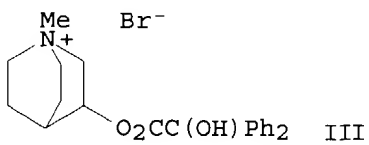
L7 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1979:136833 CAPLUS
DN 90:136833
TI Sources of error and criteria for the selection of internal standards for quantitative mass spectrometry. Part II
AU Millard, Brian J.
CS Div. Drug Chem., Food and Drug Adm., Washington, DC, USA
SO GC-MS News (1978), 6(6), 80-5
CODEN: GMNEDS; ISSN: 0388-1288
DT Journal
LA English
GI



I



II



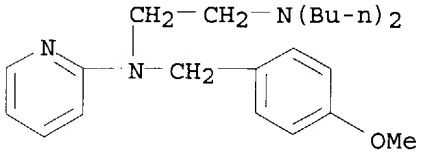
III

AB Internal stds. for quant. mass spectrometry may be stable isotope labeled analogs of the compound of interest, homologs of that compound, or compds. from the same chemical class as the compound of interest. For example, I is used as the internal standard in the measurement of the impurity II in anal. of clidinium bromide (III).

IT **69569-89-7**
RL: PRP (Properties)
(mass spectrum of, in presence of analog)

RN 69569-89-7 CAPLUS

CN 1,2-Ethanediamine, N,N-dibutyl-N'-[(4-methoxyphenyl)methyl]-N'-2-pyridinyl- (9CI) (CA INDEX NAME)



L7 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1972:405140 CAPLUS

DN 77:5140

TI Antihistaminic monoalkyl-substituted diarylamino- and aryl [(4-alkylbenzyl)amino]alkylamines

IN Cross, Peter E.; Leeming, Peter R.

PA Pfizer Corp.

SO Ger. Offen., 21 pp.
CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 2141795	A	19720302	DE 1971-2141795	19710820
	GB 1306450	A	19730214	GB 1970-40514	19700822
	BE 771152	A1	19720210	BE 1971-106924	19710810
	FR 2103448	A1	19720414	FR 1971-30402	19710820
	FR 2103448	A5	19720414		
PRAI	GB 1970-40514		19700822		

GI For diagram(s), see printed CA Issue.

AB The amines (I) [R = Et, Me; R1 = Me3C, Me3CCH2; (NR2) = piperidino, 1-pyrrolidinyl, tetrahydro-1H-azepin-1-yl; n = 1,2,3; m = 0] were prepared from p-Me3CC6H4NHPh by treatment with Cl(CH2)nNR2 in the presence of NaH. Similarly prepared were other I [R = Et, Pr, Me; R1 = Me3C, Me3CCH2; (NR2) = tetrahydro-1H-azepin-1-yl, 1-pyrrolidinyl; n = 2, m = 1].

IT **36716-54-8P 36735-45-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

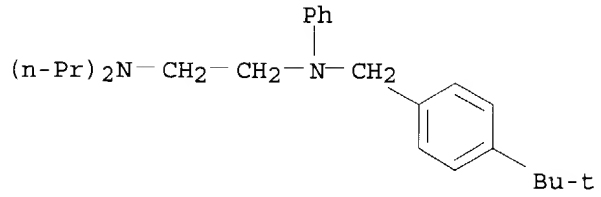
RN 36716-54-8 CAPLUS

CN 1,2-Ethanediamine, N-[[4-(1,1-dimethylethyl)phenyl]methyl]-N-phenyl-N',N'-dipropyl-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

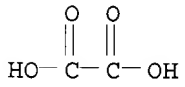
CRN 47552-17-0
CMF C25 H38 N2

765



CM 2

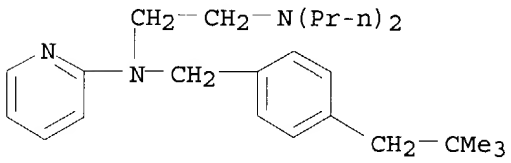
CRN 144-62-7
CMF C2 H2 O4



RN 36735-45-2 CAPLUS
CN 1,2-Ethanediamine, N-[[4-(2,2-dimethylpropyl)phenyl]methyl]-N',N'-dipropyl-N-2-pyridinyl-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

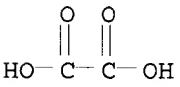
CM 1

CRN 47589-32-2
CMF C25 H39 N3



CM 2

CRN 144-62-7
CMF C2 H2 O4



L7 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1970:78788 CAPLUS
DN 72:78788
TI Chemotherapy with fluorinated compounds. II. Fluorinated aromatic derivatives of ethylene diamine
AU Maziere, Mariannick; Maziere, Bernard; Ta-Thu-Cuc; Nyugen-Dat-Xuong
CS Inst. Chem. Subst. Natur., CNRS, Gif-sur-Yvette, Fr.
SO Chimica Therapeutica (1969), 4(5), 349-52
CODEN: CHTPBA; ISSN: 0009-4374
DT Journal

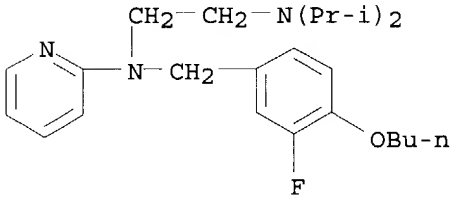
LA French

AB Twelve fluorinated aromatic ethylenediamine derivs. (2-C5H4N)(ArCH2)NCH2CH2-NR2 (I) were prepared by condensation of fluoroalkoxybenzaldehydes with 2-aminopyridine, reduction of the resulting Schiff base with HCO2H, and condensation of the resulting secondary amine with ClCH2CH2NR2. I prepared were (Ar, R, b.p./mm, and n20D given): 3,4-F(PrO)C6H3, Et, 179°/0.35, 1.5408; 3,4-F(PrO)-C6H3, iso-Pr, 188°/0.4,1.5385; 3,4-F(PrO)C6H3, Bu, 212°/0.7, 1.5313; 3,4-F(BuO)C6H3, Et, 175°/0.03, 1.5424; 3,4-F(BuO)-C6H3, iso-Pr, 193°/0.35,1.5368; 3,4-F(BuO)C6H3, Bu, 200°/0.25, 1.5280; 2,5-(PrO)FC6H3, Et, 170°/0.25, 1.5433; 2,5-(PrO)FC6H3, iso-Pr, 175°/0.25,1.5373; 2,5-(PrO)FC6H3, Bu, 179°/0.03, 1.5287; 2,5-(BuOFC6H3, Et, 168°/0.15, 1.5451; 2,5-(BuO)FC6H3, iso-Pr, 168°/0.03, 1.5328; and 2,5-(BuO)FC6H3, Bu, 186°/0.2, 1.5259. These compds. were evaluated for local anesthetic, antihistamine, and antimicrobial activity.

IT **24740-94-1 24740-95-2 25472-18-8 25472-20-2 25472-23-5 25472-24-6 26593-26-0 26593-27-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(chemotherapeutic activity)

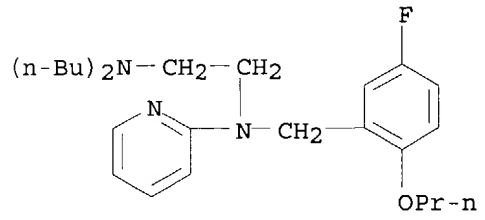
RN 24740-94-1 CAPLUS

CN 1,2-Ethanediamine, N-[(4-butoxy-3-fluorophenyl)methyl]-N',N'-bis(1-methylethyl)-N-2-pyridinyl- (9CI) (CA INDEX NAME)



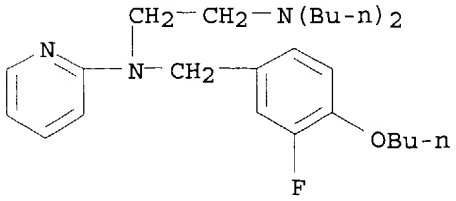
RN 24740-95-2 CAPLUS

CN 1,2-Ethanediamine, N,N-dibutyl-N'-[(5-fluoro-2-propoxyphenyl)methyl]-N'-2-pyridinyl- (9CI) (CA INDEX NAME)



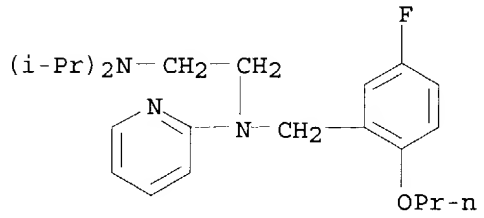
RN 25472-18-8 CAPLUS

CN Pyridine, 2-[(4-butoxy-3-fluorobenzyl)[2-(dibutylamino)ethyl]amino]- (8CI) (CA INDEX NAME)

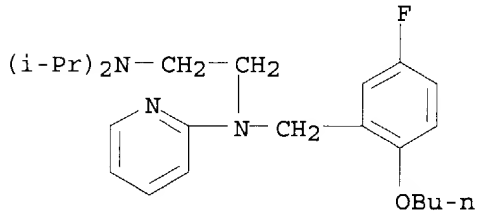


765

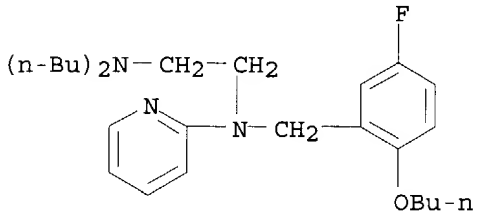
RN 25472-20-2 CAPLUS
CN Pyridine, 2-[[2-(diisopropylamino)ethyl](5-fluoro-2-propoxybenzyl)amino]-
(8CI) (CA INDEX NAME)



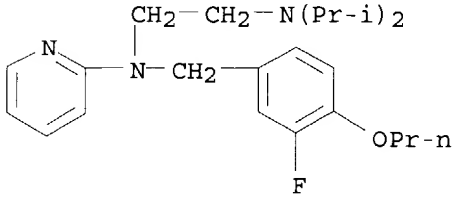
RN 25472-23-5 CAPLUS
CN Pyridine, 2-[(2-butoxy-5-fluorobenzyl)[2-(diisopropylamino)ethyl]amino]-
(8CI) (CA INDEX NAME)



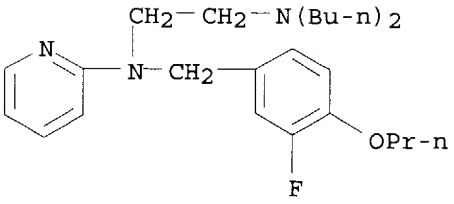
RN 25472-24-6 CAPLUS
CN Pyridine, 2-[(2-butoxy-5-fluorobenzyl)[2-(dibutylamino)ethyl]amino]- (8CI)
(CA INDEX NAME)



RN 26593-26-0 CAPLUS
CN Pyridine, 2-[[2-(diisopropylamino)ethyl](3-fluoro-4-propoxybenzyl)amino]-
(8CI) (CA INDEX NAME)



RN 26593-27-1 CAPLUS
CN Pyridine, 2-[[2-(dibutylamino)ethyl](3-fluoro-4-propoxybenzyl)amino]-
(8CI) (CA INDEX NAME)

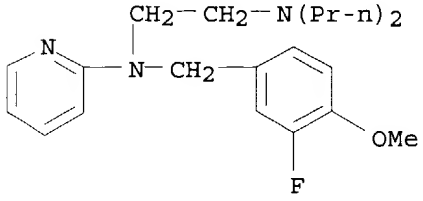


L7 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1968:443880 CAPLUS
DN 69:43880
TI Fluorine chemotherapy: new aromatic fluorinated derivatives of ethylenediamine
AU Maziere, B.; Dat-Xuong, N.
CS Inst. Chim. Subst. Natur., C.N.R.S., Gif-sur-Yvette, Fr.
SO Chim. Ther. (1968), 3(1), 1-9
CODEN: CHTQAC
DT Journal
LA French
GI For diagram(s), see printed CA Issue.
AB I, where R1 or R3 is F, are prepared and converted into the corresponding II. III, IV, and V are also prepared Thus, HCl gas is introduced into a mixture of 60 g. o-MeC6H4F, 200 ml. ether, 88 ml. 40% H2CO, 10 g. ZnCl2, and 1 g. NaCl at 20-5° to give 85% 3-fluoro-4-methoxy-α-chlorotoluene (VI), b13 122°, m. 36° (pentane). Similarly prepared are the following I [R, R1, R2, R3, b.p./mm., nD (temperature) and % yield given]: H, F, EtO, H, 130°/17, 1.524 (20°), 70; H, F, PrO, H, 140°/16, 1.513 (23°), 68; H, F, BuO, H, 145°/13, 1.509 (21°), 60; MeO, H, H, F, 106°/10, - [m. 50° (heptane)], 78; EtO, H, H, F, 113°/11, 1.510 (22°), 66; PrO, H, H, F, 134°/20, 1.504 (22°), 65; and BuO, H, H, F, 114°/17, 1.502 (23°), 57. A mixture of 44 g. VI and 35.3 g. hexamethylenetetramine in 110 ml. CHCl3 is refluxed 1 hr. and worked up to give 69% 3-fluoro-4-methoxybenzaldehyde (VII), m. 31°; 2,4-dinitrophenylhydrazone m. 199°; thiosemicarbazone m. 194°. Similarly prepared are the following II (R, R1, R2, R3, b.p./mm., m.p., m.p. thiosemicarbazone, and % yield given): H, F, EtO, H, 138°/13, 29°, 191°, 50; H, F, PrO, H, 142°/14 (n22D 1.530), -, 173°, 35; H, F, BuO, H, 150°/13 (n21.5D 1.523), -, 156°, 30; MeO, H, H, F, 118°/14, 47°, 224°, 47; EtO, H, H, F, 130°/14, 48°, 216°, 49; PrO, H, H, F, 141°/20, 30°, 163°, 36; and BuO, H, H, F, 145°/13 (n25D 1.508), -, 150°, 31. A solution of 1.10 g. VII thiosemicarbazone, 1.20 g. ClCH2CO2H, and 2 g. NaOAc in 20 ml. EtOH is refluxed 1 hr. to give III (R = R3 = H, R1 = F, R2 = MeO), m. 302°. Similarly prepared are the following III (R, R1, R2, R3, and m.p. given): H, F, EtO, H, 258°; H, F, PrO, H, 242°; H, F, BuO, H, 217°; MeO, H, H, F, 269°; EtO, H, H, F, 240°; PrO, H, H, F, 231°; and BuO, H, H, F, 228°. The following IV (Ar = 2-pyridyl) were prepared (R, R1, R2, R3, m.p., and % yield given): H, F, MeO, H, 113°, 75; H, F, EtO, H, 88.5°, 78; H, F, PrO, H, 75°, 71; H, F, BuO, H, 62.5°, 68; MeO, H, H, F. 77°, 80; EtO, H, H, F, 77.5°, 85; PrO, H, H, F, 70°, 72; and BuO, H, H, F, 58°, 70. The following IV (Ar = 2-pyrimidyl) were prepared (R, R1, R2, R3, m.p., and % yield given): H, F, MeO, H, 91.5°, 85; H, F, EtO, H, 107° 83; MeO, H, H, F, 92°, 82; and EtO, H, H, F, 102.5°, 80. [IV were prepared according to A. E. Chichibabin and I. L. Knunyants (1931)]. IV are treated with LiNH2 and the lithio derivs.

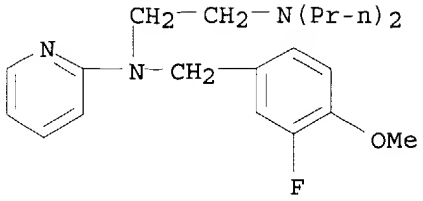
obtained are condensed with compds. of the formula ClCH2CH2NR42 to give N-(3-fluoro-4-methoxybenzyl)-N-(2-pyridyl) -N', N'-dimethylethylenediamine (b0.09 63°, n22D 1.568; HCl salt m. 145°, di-HCl salt m. 114°) and the following V (Ar = 2-pyridyl) [R, R1, R2, R3, R4 or NR42, b.p./mm., nD (temperature), m.p. HCl salt, and m.p. di-HCl salt given]: H, F, MeO, H, Et, 178°/0.09, 1.558 (22°), 128°, 110°; H, F, MeO, H, iso-Pr, 188°/0.2, 1.548(22°), 140°, 117°; H, F, MeO, H, piperidino, 202°/0.2, 1.573(20.5°), 165°, 124°; H, F, MeO, H, morpholino, 208°/0.2, 1.575 (20°), 158.5°, 139°; H, F, EtO, H, Me, 161°/0.4, 1.560(23°), 144°, 108°; H, F, EtO, H, Et, 180°/0.1, 1.550(22°), 127°, 115°; H, F, PrO, H, Me, 170°/0.5, 1.556(19.5°), 116.5°, 76°; H, F, BuO, H, Me, 182°/0.5, 1.551(22°), 108°, -; MeO, H, H, F, Me, 163°/0.1, 1.565(25°), 174°, 143°; MeO, H, H, F, Et, 166°/0.1, 1.553(23°), 138.5°, 121°; MeO, H, H, F, iso-Pr, 171°/0.5, 1.544(22°), 143°, 122°; MeO, H, H, F, piperidino, 182°/0.4, 1.569(22°), 179°, 126.5°; MeO, H, H, F, morpholino, 200°/0.6, 1.571(21°), 171°, 138°; EtO, H, H, F, Me, 159°/0.6, 1.557(26.5°), 152°, 116°; EtO, H, H, F, Et, 169°/0.5, 1.547(21°), 118°, -; PrO, H, H, F, Me, 164°/0.6, 1.554(22°), 114°, -; and BuO, H, H, F, Me, 171°/0.5, 1.553(19°), 105°, -. The following V (Ar = 2-pyrimidyl) were prepared (same data given): H, F, MeO, H, Me, 160°/0.2, 1.556(22.5°), 114.5°, 77.5°; H, F, MeO, H, Et, 170°/0.2, 1.550(22°), 105.5°, 65°; H, F, EtO, H, Me, 160°/0.5, 1.558(22°), 144°, 93°; H, F, EtO, H, EtO, H, Et, 170°/0.5, 1.542(21°), 100°, -; MeO, H, H, F, Me, 150°/0.5, 1.558(22.5°), 178°, 153.3°; MeO, H, H, F, Et, 158°/0.4, 1.544(22.5°), 147°, -; EtO, H, H, F, Me, 151°/0.1, 1.558(23.5°), 158°, 145°; and EtO, H, H, F, Et, 166°/0.1, 1.540(23°), 142°, 130°.

IT **19409-40-6P 19409-41-7P 19409-42-8P 19409-75-7P 19409-76-8P 19423-08-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 19409-40-6 CAPLUS
CN Pyridine, 2-[[2-(dipropylamino)ethyl](3-fluoro-4-methoxybenzyl)amino]-(8CI) (CA INDEX NAME)

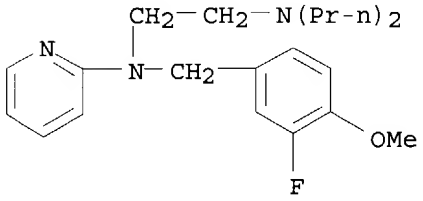


RN 19409-41-7 CAPLUS
CN Pyridine, 2-[[2-(dipropylamino)ethyl](3-fluoro-4-methoxybenzyl)amino]-, monohydrochloride (8CI) (CA INDEX NAME)



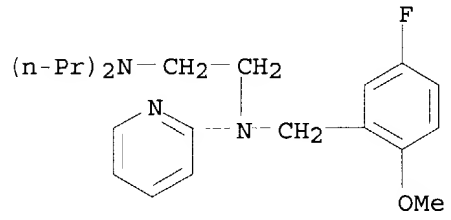
● HCl

RN 19409-42-8 CAPLUS
CN Pyridine, 2-[[2-(dipropylamino)ethyl](3-fluoro-4-methoxybenzyl)amino]-, dihydrochloride (8CI) (CA INDEX NAME)

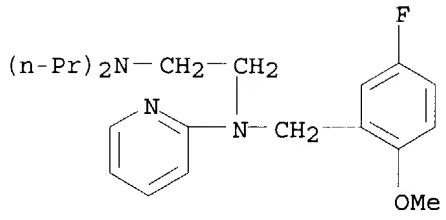


●2 HCl

RN 19409-75-7 CAPLUS
CN Pyridine, 2-[[2-(dipropylamino)ethyl](5-fluoro-2-methoxybenzyl)amino]- (8CI) (CA INDEX NAME)

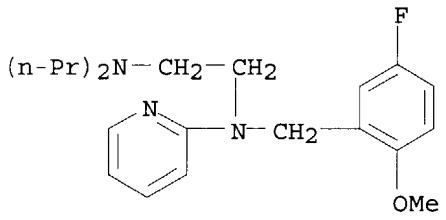


RN 19409-76-8 CAPLUS
CN Pyridine, 2-[[2-(dipropylamino)ethyl](5-fluoro-2-methoxybenzyl)amino]-, monohydrochloride (8CI) (CA INDEX NAME)



● HCl

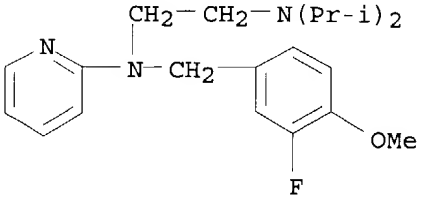
RN 19423-08-6 CAPLUS
CN Pyridine, 2-[[2-(dipropylamino)ethyl](5-fluoro-2-methoxybenzyl)amino]-, dihydrochloride (8CI) (CA INDEX NAME)



●2 HCl

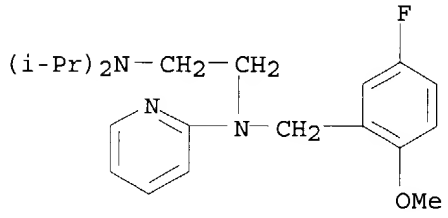
L7 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1968:409492 CAPLUS
DN 69:9492
TI Local anesthetic activity of fluoro derivatives of tetrasubstituted ethylenediamine
AU Quevauviller, Andre; Maziere, B.; Maziere, M.
CS Fac. Pharm., Paris, Fr.
SO Anesthesie, Analgesie, Reanimation (1968), 25(1), 53-9
CODEN: AAREAV; ISSN: 0003-3014
DT Journal
LA French
AB Twenty-six fluorinated, tetrasubstituted ethylenediamines were tested for local anesthetic activity on the rabbit cornea, at 5 + 10-5 moles/ml. N-(5-Fluoro-2-butoxybenzyl)-N-(2-pyrimidinyl)-N', N'-dimethylethylenediamine (I) was the most active compound (2-fold more active than procaine); all the derivs. had some activity, except N-(5-fluoro-2-ethoxybenzyl)-N-(2-pyrimidinyl)-N', N'-dimethylethylenediamine. No relation was found between the intensity of the anesthetic activity and the pH, surface tension activities, or the antihistamine activity of the test compds.; I had only weak antihistamine activity, while N-(3-fluoro-4-ethoxybenzyl)-N-(2-pyrimidinyl)-N', N'-dimethylethylenediamine, which has high antihistamine activity, had only a weak anesthetic activity.
IT **19448-06-7 19448-13-6**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(anesthetic activity of)

RN 19448-06-7 CAPLUS
CN Pyridine, 2-[[2-(diisopropylamino)ethyl](3-fluoro-4-methoxybenzyl)amino]-, monohydrochloride (8CI) (CA INDEX NAME)



● HCl

RN 19448-13-6 CAPLUS
CN Pyridine, 2-[[2-(diisopropylamino)ethyl](5-fluoro-2-methoxybenzyl)amino]-, monohydrochloride (8CI) (CA INDEX NAME)

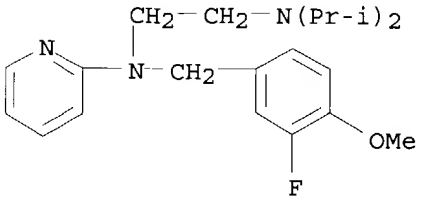


● HCl

L7 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1968:94500 CAPLUS
DN 68:94500
TI Antihistamine and antispasmodic activities and toxicity of fluorinated derivatives of ethylenediamine
AU Maziere, Bernard; Maziere, Mariannick
CS Lab. Hyg. Educ. Sanit., Fac. Pharm. Paris, Paris, Fr.
SO Chim. Ther. (1967), 2(5), 336-42
CODEN: CHTQAC
DT Journal
LA French
GI For diagram(s), see printed CA Issue.
AB Antihistaminic and antispasmodic activities and toxicities are examined for 26 fluorinated derivs. of ethylenediamine having the formula I, where R = Me, Et, iso-Pr or NR2 = piperidino or morpholino, X = CH or N, and R1 ± Me, Et, Pr, or Bu. The introduction of 1 atom of F is accompanied by a decrease in antihistaminic activity, an increase in musculotropic spasmolytic properties, and no change in acute toxicity. Lengthening the alkoxy radical proportionally decreases the acute toxicity, but is accompanied also by a decrease in antihistaminic activity.
IT **19448-06-7 19448-13-6**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(antihistaminic and antispasmodic activity of)

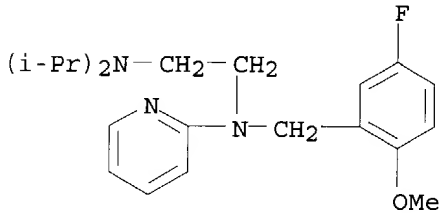
765

RN 19448-06-7 CAPLUS
CN Pyridine, 2-[[2-(diisopropylamino)ethyl](3-fluoro-4-methoxybenzyl)amino]-, monohydrochloride (8CI) (CA INDEX NAME)



● HCl

RN 19448-13-6 CAPLUS
CN Pyridine, 2-[[2-(diisopropylamino)ethyl](5-fluoro-2-methoxybenzyl)amino]-, monohydrochloride (8CI) (CA INDEX NAME)



● HCl

=>